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Implicit *FWHM* calibration for gamma-ray spectra

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Abstract *FWHM* calibration is one of the essential procedures in gamma-ray spectra analysis. Traditional method is time consumption and poor flexibility because of extra measurement on calibration source. This paper introduces an implicit calibration method based on symmetric zero-area conversion. The single peaks can be differentiated from doublets. Meanwhile, the extracted *FWHM* values can be applied in the fitting process. Various forms of calibration equations are introduced and compared with practical spectrum data under this method.

Key words Gamma-ray spectrum, *FWHM*, Implicit calibration, Symmetric zero-area conversion

1 Introduction

The particular measure of the peak widths in gamma-ray spectrometry, *FWHM* (Full width at half maximum), indicates the resolution of the gamma spectroscopy system. The *FWHM* expressed in keV has a relationship with energy of incident gamma-ray.

It is important to know the *FWHM* of peaks as an energy function when analyzing gamma spectra, especially in peak searching and fitting[1]. Thus, an accurate *FWHM* calibration needs be performed as the basis of spectrum processing.

2 Physical essence of *FWHM*

Gamma-ray spectrum is actually the energy response of the detection system to the gamma-rays of particular energies. Peaks in the spectrum are spread over several channels that can be characterized as a Gaussian distribution, whose standard deviation can be predicted by[2]

$$\sigma^2=\sigma^2_I+\sigma^2_P+\sigma^2_C+\sigma^2_E \quad (1)$$

σ is the overall uncertainty of the peak in the spectrum in energy form.

σ_I is the intrinsic width of nuclear energy levels, which is extremely smaller than σ, and can be ignored[2].

σ_P is the statistical fluctuation of the production of electron-hole pairs (n) in the detector. The number of electron-hole pairs created by a gamma-ray of energy (E) subjects to Fano distribution (F)[3]. On defining "W" as the average energy consumption to create a pair, the expected uncertainty of n is $\sigma_n=(F\times n)^{0.5}=[(F\times E)/W)]^{0.5}$.

σ_C is the uncertainty in collecting the charge by the detector caused by trapping effect. Due to the complexity effect, there is no a simple way to express the uncertainty as an energy function[3]3. However, a linear relationship of $\sigma_C=cE$ appears to be satisfactory, but not theoretical reason[2].

σ_E, the contribution from electronic noise in pulse processing system, is performed as a constant to the gamma-rays with any energy.

3 *FWHM* calibration equations[2]

There are mainly three independent effects in influencing the resolution of gamma-ray spectrum. Using the energy form ΔE to express the *FWHM* of a Gaussian-shaped peak in the spectrum, we can give

$$\Delta E\approx 2.355\sigma^{[3]}$$

Or

$$\Delta E^2=(p^2E)+(cE)^2+e^2 \quad (2)$$

where p, c, and e are constant related to fluctuation, collection, and electronic noise, respectively.

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The square root for both side of Eq.(2) is taken, And

$$\Delta E = \sqrt{\mathrm{p}^2 E + \mathrm{c}^2 E^2 + \mathrm{e}^2} = \sqrt{a_0^2 + a_1^2 E + a_2^2 E^2} \quad (3)$$

Debertin and Helmer[4] introduced Eq.(4) by ignoring the factor of incomplete charge collection.

$$\Delta E = \sqrt{\mathrm{p}^2 E + \mathrm{e}^2} = \sqrt{a_0^2 + a_1^2 E} \quad (4)$$

In addition, Eq.(5) with simpler expression can be found in the commercial programs of Genie 2000[5].

$$\Delta E = a_0 + a_1 \sqrt{E} \quad (5)$$

Gilmore conducted a series of experiments to compare the fitting *FWHM* calibrations with different formulae[2] (Table 1). The best fit is from the square root quadratic function, and a simple quadratic fit. The Genie 2000 fitting is worse than the linear equation.

Table 1 Results of fitting *FWHM* data to different functions[2]

Fitting type	Formulae	RMS differences
Linear	a_0+a_1E	0.020
Quadratic	$a_0+a_1E+a_2E^2$	0.0065
Genie 2000	$a_0+a_1E^{0.5}$	0.055
Debertin and Helmer	$(a_0^2+a_1^2E)^{0.5}$	0.026
Square root quadratic	$(a_0+a_1E+a_2E^2)$	0.0057

4 Traditional *FWHM* calibration

Similar to energy calibration, traditional *FWHM* calibration method is accomplished by measuring gamma-rays of precisely known energy and estimating the relationship between the peak width and energy[1].

The three ways can provide proper gamma-ray emission source. (1) Several kinds of nuclides with single or discrete energies are chosen and mixed together; (2) One specific nuclide emitting a variety of energies is chosen, covering the entire range of the spectrum, such as ^{152}Eu. The known nuclides in the test sample can be used to perform the calibration.

Explicit method can be used to fine calibration; but its calibration source needs be additionally measured by time consumption. Especially, when changing experiment condition, the spectroscopy should be recalibrated by employing a new measurement except applying for nuclides in any situation. In this paper, an implicit method for *FWHM* calibration is developed by self-information gained from the target spectrum.

5 Implicit *FWHM* calibration method

5.1 Method introduction

The Ge(Li) detector has high energy resolution, and makes a great number of gamma peaks with enough distance each other, separating single peaks easily.

Implicit method contains two calibration procedures. First, single peaks are examined and extracted from the spectrum. Second, the width of each singlet is calculated. Together with the peak position, the calibration curve is obtained by fitting these data.

Comparing all kinds of peak searching algorithms with implicit *FWHM* calibration, symmetric zero-area conversion method (SZA) has advantages in low noise sensitivity, fine multi-peaks resolving and weak peak identifying abilities[1].

5.2 Method description

The spectrum data are convoluted by the SZA method using a zero-area window. The linear base tends to zero after convolution while maximum value is at the positions of gamma peaks. The conversion process is described as Eq.(6).

$$\tilde{y}_i = \sum_{j=-m}^{m} C_i y_{i+j} \qquad \sum_{j=-m}^{m} C_j = 0 \qquad C_j = C_{-j} \quad (6)$$

where y_i and $\tilde{y}_i$ are the spectrum data before and after conversion, and C_j is the window coefficient.

Among various forms of window functions, Gaussian second derivative has the best property[6], its coefficients can be expressed as Eq.(7).

$$W(j) = C_j = \frac{1}{\sigma_w^4}(j^2 - \sigma_w^2)\exp\left[-\frac{1}{2}(j/\sigma_w)^2\right] \quad (7)$$

where, σ_w is the standard deviation from the original Gaussian distribution $G_w(j)$.

Figure 1 shows a Gaussian second derivative formed SZA window function with σ_w=4.

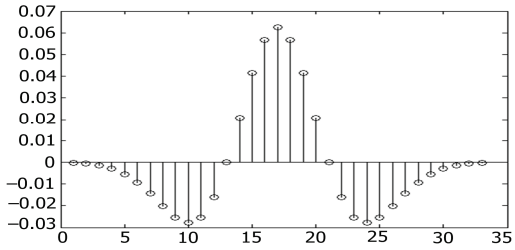

Fig.1 Gaussian second derivative formed SZA window function.

And, gamma peaks in the spectrum can be treated as Gaussian shape approximately.

$$G_\gamma(i) = y_i = H\exp\left[\frac{(i-p)^2}{2\sigma_\gamma^2}\right] \tag{8}$$

where, H, p and σ_γ are their amplitude, position and standard deviation, respectively.

Due to the convolution nature[7], a Gaussian peak conversion operated with the window function maintains the appearance of Gaussian second derivative, as shown in Fig.2.

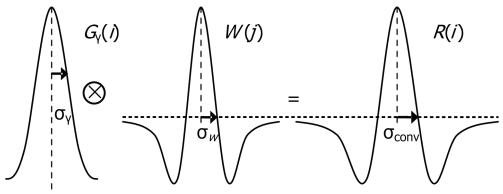

Fig.2 Convolution between Gaussian peak and window function.

$$R(i)=G_\gamma(i)\times W(j) = G_\gamma(i)\times G_w(j)''$$
$$=[G_\gamma(i)\times G_w(j)]=G_{conv}(i)'' \tag{9}$$

$G_{conv}(i)$ is the convolution of gamma peak and the original Gaussian distribution of the window which has a Gaussian form of $\sigma_{conv}=(\sigma^2_w\sigma^2_\gamma)^{0.5}$.

The distance between two zero-crossing points beside the conversion maximum can be obtained from the Gaussian second derivation.

$$D=2\sigma_{conv}=2(\sigma^2_w+\sigma^2_\gamma)^{0.5} \tag{10}$$

The σ_γ of the gamma peak is deduced from intercept D and σ_w, subsequently, the peak *FWHM* is expressed by Eq.(11).

$$FWHM \cong 2.355\sigma_\gamma = 2.355\sqrt{(D^2/4)-\sigma_w^2} \tag{11}$$

The Eq.(11) is only valid for single peaks, and the calculated *FWHM* is definitely a constant for every pair of D and σ_w. While for multi-peaks, the intercept D relates to the intervals and ratios between the component peaks, in other words, the *FWHM* obtained from Eq.(11) is meaningless.

Consequently, the same spectrum can be converted using several windows with different σ_w. When the *FWHM* value tends to be invariable, the corresponding peak is considered as a singlet, thus distinguishing a set of multi-peaks due to their invalid *FWHM*. Also, the *FWHM* of each single peak can be gained, implementing the *FWHM* calibration process.

5.3 Method modification

Applying to practical spectra, a group of simulation data set up is used to test the calibration method.

The σ_w of 8 window functions equal to 1 to 8 is convoluted by σ_γ of 4 individual Gaussian peaks equal to 1, 2, 4, and 8. The calculated and theoretical *FWHM* values are compared (Table 2, Fig.3).

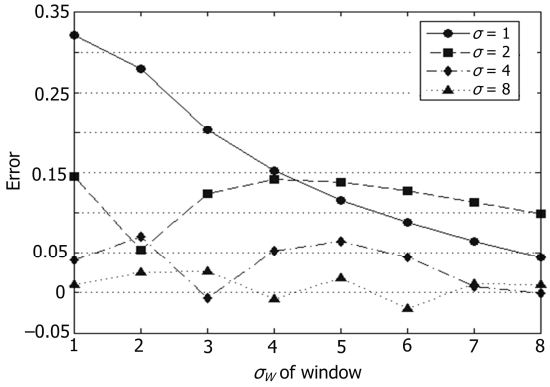

Fig.3 Error between the calculated and theoretical *FWHM* values under different windows.

Table 2 Difference between calculated *FWHM* and theoretical value

σ_γ	Theoretical *FWHM*	Error between calculated and theoretical *FWHM* values									
		σ_w=1	σ_w=2	σ_w=3	σ_w=4	σ_w=5	σ_w=6	σ_w=7	σ_w=8	Mean	Std
1	2.355	0.321	0.279	0.204	0.152	0.116	0.0881	0.0650	0.0445	0.159	0.101
2	4.710	0.146	0.0542	0.124	0.142	0.139	0.127	0.114	0.0992	0.118	0.0301
4	9.419	0.0405	0.0700	–0.00681	0.0527	0.0646	0.0442	0.00736	$-1.71e^{-4}$	0.0340	0.0299
8	18.84	0.00967	0.0258	0.0263	–0.00798	0.0177	–0.0202	0.0114	0.0102	0.00912	0.0161

To reduce the difference in Eq.(11), a modification factor is introduced to Eq.(12).

$$FWHM \cong 2.355\sqrt{(D^2/4)-\sigma_w^2-(a/\sqrt{\sigma_w})} \qquad (12)$$

The constant (a) is determined by applying an iteration method to optimize the average error under every window function for each Gaussian peak.

Figure 4 shows the result using Eq.(12). Under every window with different σ_w, the mean of residual errors approaches to zero, and the fluctuation is suppressed at some levels.

In practical application, the σ_w values should be selected. The SZA method can separate multipeaks with small σ_w, but is sensitive to the noise. On the other hand, the reliable window of large σ_w is inadequate in multipeak processing. For σ_w, a value approximating to σ_γ suggests obtaining the optimal results. Therefore, σ_w can be determined within a rough range related to *FWHM* varying in the spectrum. Also, this method is compared with calculation process. The average background level above and below the peak is subtracted from the estimated peak height to get the expected count. The two positions of half height on the peak are obtained by linear interpolation, and the distance is exactly the *FWHM*. The resultant reliability depends on the uncertainty of peak height and background level.

Quadratic formed background and noise with constant SNR are added to a Gaussian peak by σ_γ=4 to simulate an actual gamma peak. The 100 sets of simulation data with random background and noise are processed by the two methods (Table 3).

The *FWHM* calculated by Eq.(12) approximates to the theoretical value. For the direct approach, the result is relatively fluctuant due to the noise. Applied first to reduce the standard deviation, a smoothing process impacts the FWHM value to a certain extent.

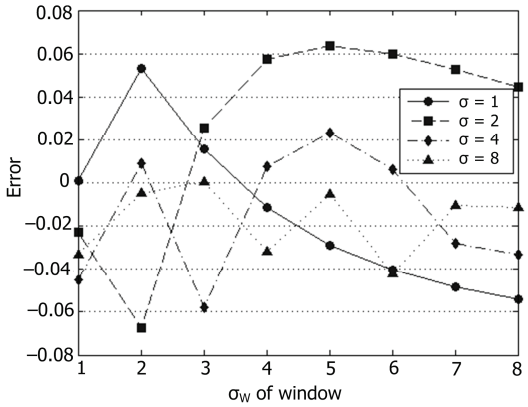

Fig.4 Error between calculated and theoretical *FWHM* values Eq.(12).

Table 3 Compare of direct process and method in this paper

Method	Theoretical *FWHM*	Error of 100 experiments	
		Mean	Std
Direct-without smoothing		–0.0296	0.252
Direct-with smoothing	9.419	–0.0405	0.221
This paper		0.0167	0.170

6 Method verification

A gamma-ray spectrum from sand sample is measured by HPGe detector, and used to test the implicit *FWHM* calibration method (Fig.5).

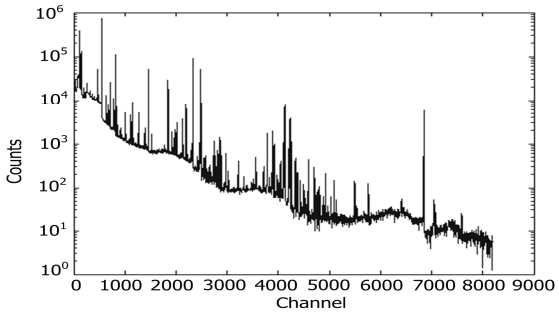

Fig.5 Practical gamma-ray spectrum.

The 3 windows with σ_w equal to 2, 3, and 4 are employed to convert the spectrum and calculate the *FWHM* corresponding to each peak, the three sets of *FWHM* deviation is applied to pick out single peaks, and their mean value is used to the fitting procedure.

HYPERMET, a mature developed γ spectrum analysis code, and Genie 2000 program are employed to validate the calculation in Table 4. The HYPERMET using a region fitting method to get accurate peak position and *FWHM* can be used as the standard value, while Genie 2000 applies a direct process to calculate *FWHM*. Together with *FWHM* values, the relative errors comparing to HYPERMET

are calculated for the other two processes, as shown in Table 5. The relative errors within ±3% are obviously better than Genie 2000 except one point. In addition, both HYPERMET and Genie program need a rough *FWHM* calibration as input to obtain proper results, while the novel method is fully automatic.

Table 4 Calculated *FWHM* and position of each single peak

Peak position	Calculated *FWHM*				
	σ_w=2	σ_w=3	σ_w=4	Mean	Std
323	2.729	2.917	2.833	2.826	0.0946
470	2.770	2.835	2.773	2.793	0.0368
631	2.990	3.111	3.110	3.070	0.0699
812	3.236	3.254	3.267	3.253	0.0153
1116	3.410	3.414	3.398	3.407	0.00824
1407	3.635	3.653	3.592	3.627	0.0312
1531	3.782	3.722	3.748	3.751	0.0301
1918	3.976	4.025	4.065	4.022	0.0443
2197	4.227	4.217	4.220	4.222	0.00494
2861	4.600	4.616	4.634	4.616	0.0169
4127	5.446	5.538	5.501	5.495	0.0460
4335	5.580	5.642	5.583	5.602	0.0347
4595	5.754	5.847	5.703	5.768	0.0728
6851	7.049	7.131	7.229	7.137	0.0901

Table 5 The *FWHM* calculated by different methods

Peak position	Calculated *FWHM*				
	HYPERMET	Genie	Relative error / %	This paper	Relative error / %
323	2.751	3.024	9.939	2.826	2.726
470	2.905	2.945	1.371	2.793	-3.855
631	3.131	3.210	2.527	3.070	-1.948
812	3.190	3.237	1.463	3.253	1.975
1116	3.368	3.396	0.8266	3.407	1.158
1407	3.660	3.688	0.7560	3.627	-0.9016
1531	3.685	3.714	0.7924	3.751	1.791
1918	4.025	4.245	5.461	4.022	-0.07453
2197	4.190	4.218	0.6747	4.222	0.7637
2861	4.588	4.457	-2.854	4.616	0.6103
4127	5.446	5.651	3.762	5.495	0.8997
4335	5.550	5.571	0.3874	5.602	0.9406
4595	5.727	6.261	9.326	5.768	0.7159
6851	7.065	7.137	1.007	7.137	1.013

Table 6 and Fig.6 show the compared position-*FWHM* data from Table 4 fitted to the 5 equations in Section 3. The square root quadratic function has the best effect, and the linear fit performs better than Genie 2000 function, this is consistent with the conclusion in Section 3.

Table 6 Compare of different equations fitting *FWHM* data

Calibration equation	RMS differences
Square root quadratic	0.0235
Quadratic	0.0285
Linear	0.0774
Debertin and Helmer	0.162
Genie 2000	0.433

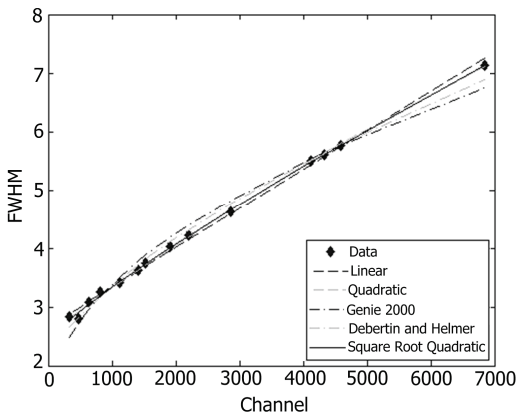

Fig.6 Fitting curves of the 5 calibration equations.

The performance of above 3 typical equations is shown in Fig.7.

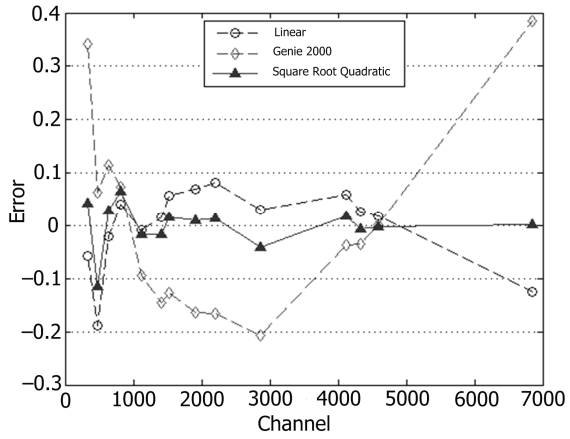

Fig.7 Error between fitted functions and *FWHM* data.

7 Conclusions

In this paper, an implicit *FWHM* calibration algorithm is introduced as a complement to traditional method. The new algorithm is developed on the basis of symmetric zero-area conversion method, and uses the self-information from the object spectrum. The method is tested, modified, and compared to a direct calculation process first using simulation data. Ultimately, this method is applied to a practical gamma-ray spectrum, and the calibration result is proved to be good.

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